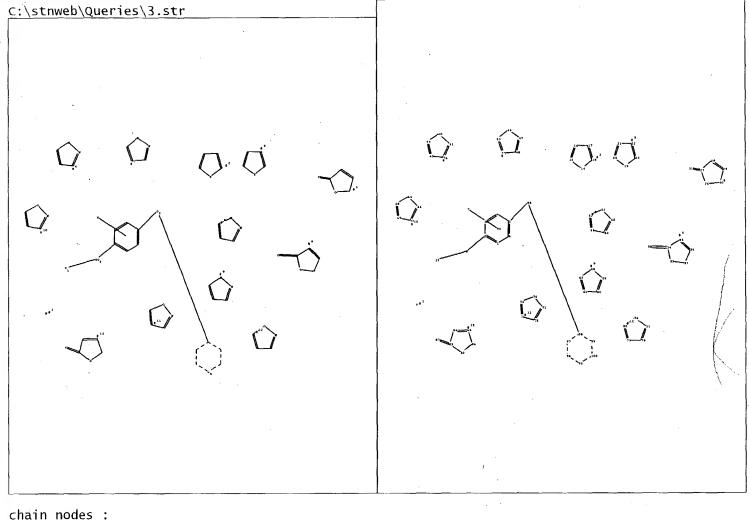


```
7 10 16 18
ring nodes:
    1 2 3 4 5 6 11 12 13 14 15
chain bonds:
    2-7 7-10
ring bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-15 12-13 13-14 14-15
exact/norm bonds:
    7-10
exact bonds:
    2-7 11-12 11-15 12-13 13-14 14-15
normalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems:
    containing 1 : 11 :
```

G1:Ak,NH2

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:Atom 19:CLASS



```
31 38 87
    7 8 9 12
ring nodes :
                   5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 14 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 95 96
                                                                                                        33 34 35
     1
         37
              40
    94 65
97 65
              66
              99
                   100
chain bonds
    2-8 5-93
                  8-12 27-31 34-38 83-87 93-98
ring bonds:
                2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
     1-2 1-6
    21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50
                                                                                     34-35
                                                                                                               40-41
                                                                                              35-36
                                                                                                       36-37
                                                                                     52-53
                                                                                                                54-55
                                                                                                       53-54
                                                                                              52-56
   55-56
                                        60-61 61-62 64-65
76-80 77-78 78-79
                                                                           65-66
                                                                                              67-68
                                                                                                       70-71
                                                                                                               70-7LA
             58-59
                               59-60
                                                                   64-68
                                                                                     66-67
                      58-62
                      73-74
                              76-77
    71-72
             72-73
                                                                   79-80
                                                                           82-83
                                                                                     82-86
                                                                                             83-84
                                                                                                       84-85
            95-100 96-97 97-98 98-99 99-100
exact/norm bonds :
     5-93 8-12 27-31 34-38 40-41 40-44 41-42 46-47 46-50 47-48 52-53 52-56 53-54
     58-59 58-62 59-60 65-66 71-72 77-78 83-87 93-98 95-96 95-100 96-97 97-98
     98-99 99-100
exact bonds :
    2-8 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 42-43 43-44 48-49 49-50 54-55 55-56 60-61 61-62 64-65 64-68 66-67 67-68 70-71 70-74 72-73 73-74 76-77 76-80 78-79 79-80 82-83 82-86 83-84 84-85 85-86
normalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
    containing 1: 14: 19: 26: 33: 40: 46: 52: 58: 64: 70: 76: 82:
```

G1:CH3,Et,[*1]
G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 83:Atom 87:CLASS 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 100:Atom

```
:\stnweb\Queries\9.str
hain nodes :
    89
          12
             31
                 38 87 93
                            101
ing nodes :
```

```
5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86
                                               48 49 50 52 53 54 55 56 58 59 60 61 62
74 76 77 78 79 80 82 83 84 85 86 95 96
   97
      98
            99
                 100
nain bonds :
  2-8 5-93 8-12 27-31 34-38 83-87 93-98
ing bonds :
                    3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18
26-27 26-30 27-28 28-29 29-30 33-34 33-37
              2-3
   1-2 1-6
                                                                                     19-20
           22-23
                                                                                   34-35
                                                                                            35-36
                                                                                                     36-37
   40-44
           41-42
                    42 - 43
                             43-44
                                                       47-48
                                      46-47
                                               46-50
                                                                48-49
                                                                          49-50
                                                                                            52 - 56
                                                                                                     53 - 54
                                                                                                              54-55
   55-56
           58-59
                    58-62
                             59-60
                                      60-61
                                               61-62
                                                        64-65
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                                                                         65-66
                                                                                            67-68
                                                                                  66-67
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                                              77-78 78-79 79-80
   71-72
                             76-77
           72-73
                    73-74
                                      76-80
                                                                         82-83 82-86
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                                                                                                    84-85
           95-100 96-97 97-98
                                      98-99 99-100
(act/norm bonds :
  5-93 8-12 27-31 34-38 40-41 40-44 41-42 46-47 46-50 47-48 52-53 52-56 53-54 58-59 58-62 59-60 65-66 71-72 77-78 83-87 93-98 95-96 95-100 96-97 97-98
  98-99
           99-100
act bonds
  2-8 14-15
                14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27 26-30
  27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 42-43 43-44 48-49 49-50 54-55 55-56 60-61 61-62 64-65 64-68 66-67 67-68 70-71 70-74 72-73 73-74 76-77 76-80 78-79 79-80 82-83 82-86 83-84 84-85 85-86
rmalized bonds :
  1-2 1-6 2-3 3-4 4-5 5-6
olated ring systems :
  containing 1: 14: 19: 26: 33: 40: 46: 52: 58: 64: 70: 76: 82:
::CH3,Et,[*1]
:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]
```

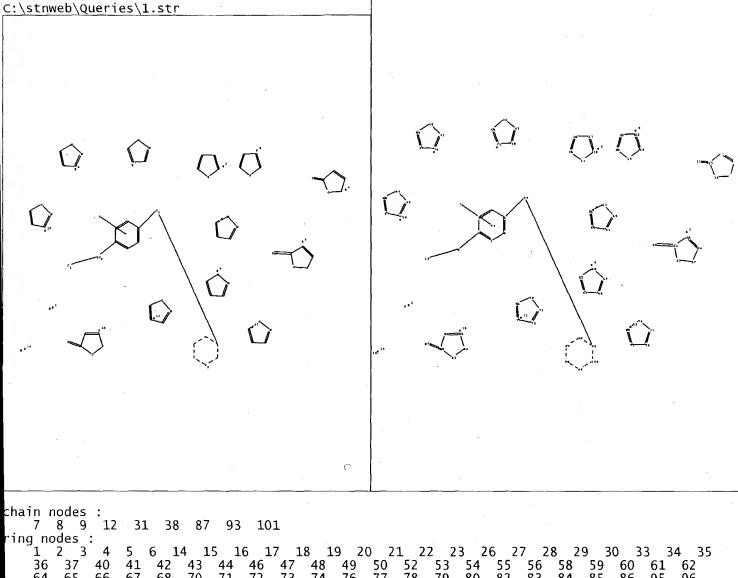
1 2

65

40

G3:C,[*14]

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 59:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom



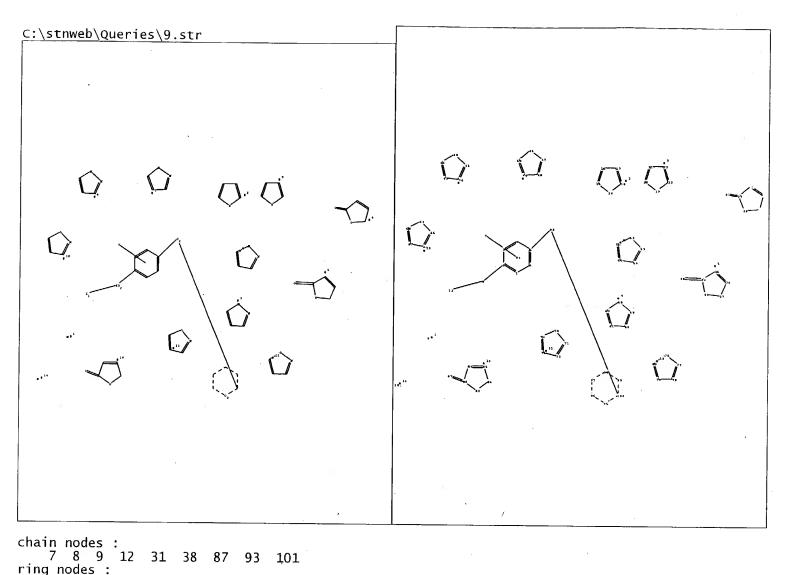
```
5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 1 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 95 96
    64
         65
            66
    97
                  100
         98
             99
chain bonds
    2-8
        5-93 8-12 27-31 34-38 83-87 93-99
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
           34-35
                                                                                       35-36
    21-22
                                                                                                36-37
                                                                                                        40-41
    40-44
                                                                               52-53
                                                                                       52-56
                                                                                                        54-55
                                                                                                53-54
                                             61-62 64-65
77-78 78-79
    55-56
                             59-60
                                                              64-68
                                                                      65-66
                                                                                       67-68
            58-59
                     58-62
                                     60-61
                                                                               66-67
                                                                                                70-71
                                                                                                        70-74
                    73-74 76-77
            72-73
    71-72
                                     76-80
                                                              79-80 82-83
                                                                               82-86
                                                                                      83-84
                                                                                                84-85
            95-100 96-97 97-98 98-99 99-100
    95-96
xact/norm bonds :
    5-93 8-12 27-31 34-38 40-41 40-44 41-42 46-47 46-50 47-48 52-53 52-56 53-54
    58-59 58-62 59-60 65-66 71-72 77-78 83-87 93-99 95-96 95-100 96-97 97-98
    98-99
            99-100
xact bonds
    2-8 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 42-43 43-44 48-49 49-50 54-55 55-56 60-61 61-62 64-65 64-68 66-67 67-68 70-71 70-74 72-73 73-74 76-77 76-80 78-79 79-80 82-83 82-86 83-84 84-85 85-86
ormalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6
solated ring systems :
    containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :
```

2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

1:CH3,Et,[*1]

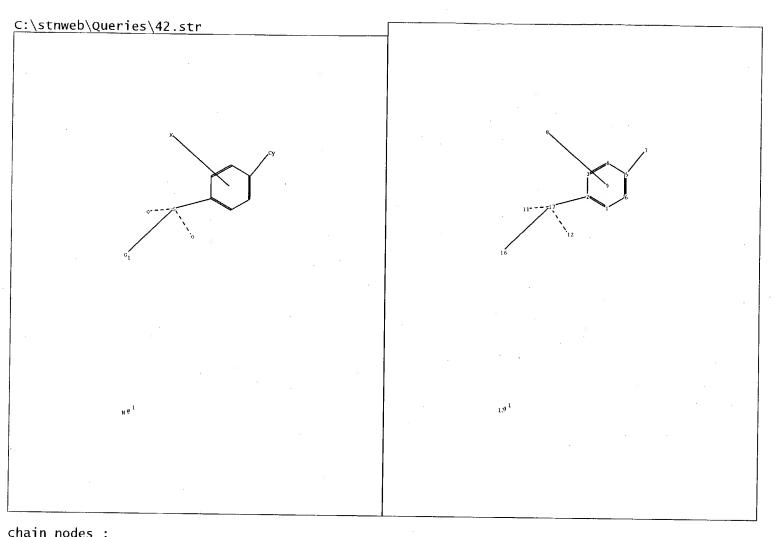
G3:C,[*14]

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 83:Atom 83:Atom 84:Atom 99:Atom 100:Atom 101:CLASS



```
41 42
67 68
      37
          40
     65
   64
         66
   97 98 99
             100
chain bonds:
   2-8 5-93 8-12 27-31 34-38 83-87 93-100
ring bonds :
           2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
   1-2 1-6
   21-22
         22-23 26-27
                    26-30
                         27-28 28-29 29-30
                                            33-34 33-37
                                                              35-36
                                                        34-35
                                                                    36-37
                                                                         40-41
              42-43
   40-44
         41-42
                    43-44
                          46-47
                                46-50
                                      47-48
                                            48 - 49
                                                 49-50
                                                        52-53
                                                              52-56
                                                                    53-54
                                                                         54-55
   55-56
         58-59
                     59-60
               58-62
                          60-61
                                                              67-68
                                61-62
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                                                                         70-74
   71-72
               73-74
         72-73
                    76-77
                          76-80
                                77-78 78-79
                                            79-80
                                                 82-83
                                                        82-86
                                                             83-84
                                                                   84-85
                                                                         85-86
   95-96
         95-100
               96-97 97-98
                           98-99 99-100
exact/norm bonds :
   5-93 8-12 27-31 34-38 40-41 40-44 41-42 46-47 46-50 47-48 52-53 52-56 53-54
         58-62 59-60 65-66 71-72 77-78 83-87 93-100 95-96 95-100 96-97 97-98
   58-59
   98-99
         99-100
exact bonds :
            14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27
   2-8 14-15
                                                                       26-30
   normalized bonds:
   1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
   containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :
G1:CH3,Et,[*1]
G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]
```

C,[*14]



```
chain nodes :
    7 8 11 12 13 16 17
ring nodes :
    1 2 3 4 5 6
chain bonds :
    2-17 5-7 11-17 12-17 16-17
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
    2-17 5-7 11-17 12-17 16-17
normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
    containing 1 :
```

G1:CH3,Et,[*1]

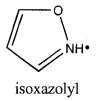
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:CLASS 9:CLASS 11:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS

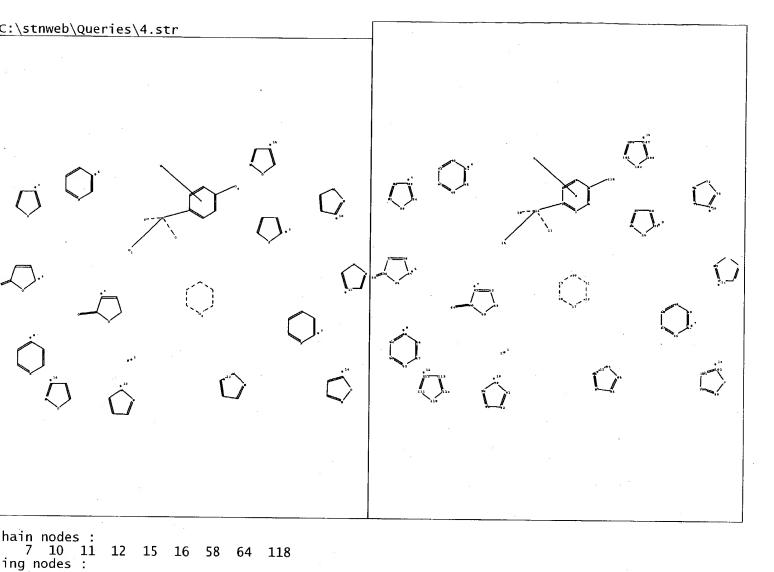
```
C:\stnweb\Queries\8.str
   7 8 11 12 13 16 17 54
ring nodes :
```

```
chain nodes :
    1 2 3 4 5 6 18 19 20 21 22 23 24 25 26 27 28 29 30 36 37 38 39 40 41 42 43 44 45 46 47
                                                                                       31
chain bonds :
     2-17 5-7 7-54 11-17 12-17 16-17
ring bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23 24-25 24-29 25-26 26-27 27-28 28-29 30-31 30-35 31-32 32-33 33-34 34-35 36-37 36-41 37-38 38-39 39-40 40-41 42-43 42-47 43-44 44-45 45-46 46-47
exact/norm bonds :
     2-17 5-7 7-54 11-17 12-17 16-17
exact bonds :
    18-19 18-23 19-20 20-21 21-22 22-23
normalized bonds:
     1-2 1-6 2-3 3-4 4-5 5-6 24-25 24-29 25-26 26-27 27-28 28-29 30-31 30-35
    31-32 32-33 33-34 34-35 36-37 36-41 37-38 38-39 39-40 40-41 42-43 42-47 43-44 44-45 45-46 46-47
isolated ring systems :
    containing 1 : 18 : 24 : 30 : 36 : 42 :
G1:CH3,Et,[*1]
```

G2:[*2],[*3],[*4],[*5],[*6]

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom
43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 54:CLASS





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      106
      107
      108
      110
      111
      112
      113
      114

     1 2 3
     37 38 39
                         40
     60 61 62
     93 94 98
hain bonds :
     2-16 5-118 10-16 11-16 15-16 36-58 60-64
ing bonds :
            1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22 25-26 25-29
     1-2
     26-27 27-28
                              28-29
                                          30-31 30-34 31-32 32-33 33-34 35-36 35-39 36-37
                                                                                                                                                     37-38
                  40-45
                               41-42
                                            42-43
                                                        43-44
                                                                     44-45
                                                                                  46-47
                                                                                               46-51 47-48
                                                                                                                          48-49
                                                                                                                                        49-50
                                                                                                                                                     50-51
                                                                                                                                                                   52-53
     52-57 53-54 54-55 55-56 56-57 59-60 59-63 60-61 61-62 62-63 72-73 74-75 75-76 78-79 78-82 79-80 80-81 81-82 84-85 84-88 85-86 86-87 90-94 91-92 92-93 93-94 98-99 98-102 99-100 100-101 101-102 104-105 105-106 106-107 107-108 110-111 110-114 111-112 112-113 113-114
                                                                                                                                                     72-76
                                                                                                                                                                  73-74
                                                                                                                                                     87-88 90-91
xact/norm bonds :
     36-58
                                                                                                             35-36 35-39
72-76 73-74
                                                                                                                                                                  37-38
                59-60 59-63 60-61 60-64 61-62 62-63 72-73 72-76 73-74 74-75 75-76 79-80 80-81 81-82 84-85 84-88 85-86 86-87 87-88 90-91 90-94 91-92 98-99 98-102 99-100 100-101 101-102 104-105 104-108 105-106 106-107
     38-39
                                                                                                                                                                  78-79
     78-82
     107-108 110-111 110-114 111-112 112-113 113-114
ormalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 40-41 40-45 41-42 42-43 43-44 44-45 46-47 46-51 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56 56-57
solated ring systems :
    containing 1 : 17 : 25 : 30 : 35 : 40 : 46 : 52 : 59 : 72 : 78 : 84 : 90 : 110 :
```

l:CH3,Et,[*1]

G4:[*1],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15],[*16]

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS 12:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:CLASS 54:CLASS 55:Atom 56:Atom 57:Atom 58:CLASS 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:CLASS 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 84:Atom 85:Atom 86:Atom 87:Atom 88:Atom 90:Atom 91:Atom 92:Atom 93:Atom 94:Atom 98:Atom 99:Atom 100:Atom 101:Atom 102:Atom 104:Atom 105:Atom 106:Atom 107:Atom 108:Atom 110:Atom 111:Atom 112:Atom 113:Atom 114:Atom 118:CLASS

```
C:\stnweb\Queries\5.str
hain nodes :
  7 9 10 11 14 15 57 63
```

```
1 2 3 4 5 6 16 17 18 19 20 21 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 58 59 60 61 62 71 72 73 74 75 77 78 79 80 81 83 84 85 86 87 89 90 91 92 93 97 98 99 100 101 103 104 105 106 107 109 110 111 112 113
hain bonds :
    2-15 5-117 9-15 10-15 14-15 21-117 35-57 59-63
ing bonds :
    \frac{1-2}{2} \frac{1-6}{2} \frac{2-3}{3} \frac{3-4}{4} \frac{4-5}{5} \frac{5-6}{6} \frac{16-17}{16-21} \frac{16-21}{17-18} \frac{18-19}{18-19} \frac{19-20}{20-21} \frac{24-25}{24-28}
    25-26 26-27 27-28 29-30 29-33 30-31 31-32 32-33 34-35 34-38 35-36 36-37 37-38
               39-44
                                     41-42
                          40-41
                                                 42-43
                                                                                  45-50 46-47
                                                            43-44 45-46
                                                                                                            47-48
                                                                                                                                  49-50
                                                                                                                      48-49
                                                                                                                                              51-52
               52~53
                                                  55-56
                           53-54
                                      54-55
                                                            58-59 58-62 59-60 60-61 61-62
                                                                                                                      71-72
                                                                                                                                  71-75
                                                                                                                                              72-73
    73-74 74-75 77-78 77-81 78-79 79-80 80-81 83-84 83-87 84-85 85-86 86-87 89-93 90-91 91-92 92-93 97-98 97-101 98-99 99-100 100-101 103-104 103-107
                                                                                                                                              89-90
    104-105 105-106 106-107 109-110 109-113 110-111 111-112 112-113
xact/norm bonds :
   2-15 5-117 9-15 10-15 14-15 16-17 16-21 17-18 18-19 19-20 20-21 21-117 24-25 24-28 25-26 26-27 27-28 29-30 29-33 30-31 31-32 32-33 34-35 34-38 35-36 35-57 36-37 37-38 58-59 58-62 59-60 59-63 60-61 61-62 71-72 71-75 72-73 73-74 74-75 77-78 77-81 78-79 79-80 80-81 83-84 83-87 84-85 85-86 86-87 89-90 89-93 90-91 91-92 92-93 97-98 97-101 98-99 99-100 100-101 103-104 103-107 104-105 105-106
    106-107 109-110 109-113 110-111 111-112 112-113
ormalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 39-40 39-44 40-41 41-42 42-43 43-44 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 55-56
solated ring systems :
   containing 1 : 16 : 24 : 29 : 34 : 39 : 45 : 51 : 58 : 71 : 77 : 83 : 89 : 109 :
```

117

ing nodes :

1:CH3,Et,[*1]

G4:[*1],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15],[*16]

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS 11:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:CLASS 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:Atom 89:Atom 90:Atom 91:Atom 92:Atom 93:Atom 97:Atom 98:Atom 99:Atom 100:Atom 101:Atom 103:Atom 104:Atom 105:Atom 106:Atom 107:Atom 109:Atom 110:Atom 111:Atom 112:Atom 113:Atom 117:CLASS 118:CLASS

```
:\stnweb\Queries\5a.str
nain nodes :
    8 9 12
               31 38 87
                           93
ing nodes :
                             16 17 18 19 20 21 22 23 26 27 28 29 30
  1 2
                 6
                        15
                   14
                                                                                   33.
              41 42 43
67 68 70
                                  47
                                      48 49 50 52 53 54 55 56 58 59 60 61 62
74 76 77 78 79 80 82 83 84 85 86 94 95
  36
          40
                          44
                              46
                                  73
     65
                              72
  64
          66
                          71
  96
     97
          98
              99
nain bonds :
             8-12 27-31 34-38 83-87 93-97
  2-8 5-93
ng bonds :
            2-3
                      4-5
  1-2 1-6
                 3-4
                           5-6 14-15 14-18 15-16 16-17 17-18
                                                                     19-20 19-23
         22-23
                26-27
                       26-30
                               27-28
                                      28-29 29-30
                                                     33-34
                                                            33-37
                                                                   34-35
                                                                           35-36
                                                                                  36-37
                                                                                         40-41
  40-44
         41 - 42
                42-43
                        43-44
                               46-47
                                      46-50
                                             47-48
                                                     48-49
                                                            49-50
                                                                   52-53
                                                                           52 - 56
                                                                                  53-54
                                                                                         54-55
  55-56
         58-59
                58-62
                        59-60
                               60 - 61
                                      61-62
                                             64-65
                                                     64-68
                                                            65-66
                                                                           67-68
                                                                                  70-71
                                                                   66-67
                                                                                         70-74
  71-72
                73-74
         72-73
                        76-77
                               76-80
                                      77-78
                                             78-79
                                                     79-80
                                                            82-83
                                                                   82-86
                                                                           83-84
                                                                                  84-85
                                                                                         85 - 86
  94-95
         94 - 99
                95-96
                       96-97
                               97-98
                                      98-99
act/norm bonds
  2-8 5-93 8-12
                   14-15
                          14-18
                                  15-16 16-17 17-18 19-20 19-23
                                                                             21-22
                                                                     20-21
  26-27
         26-30
               27-28
                       27-31
                              28-29
                                     29-30
                                             33-34
                                                     33-37
```

34 - 35

49-50

65-66

82-83

34 - 38

52-53

66-67

82-86

35 - 36

52-56

67-68

83-84

36 - 37

53-54 70-71

83-87

40-41

54-55

70-74

84-85

:CH3,Et,[*1] :[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13] :C,N

46-47

60 - 61

76-80

95-96

46-50

61-62

77-78

96-97

containing 1: 14: 19: 26: 33: 40: 46: 52: 58: 64: 70: 76: 82:

47-48

64-65

78-79

97-98

48-49

64-68

79-80

98 - 99

40-44

55-56

71-72

85-86

rmalized bonds: 1-2 1-6 2-3

41-42

58-59

72-73

93-97

olated ring systems :

42-43

58-62

73-74

94 - 95

43-44

59-60

76-77

94-99

3-4 4-5 5-6

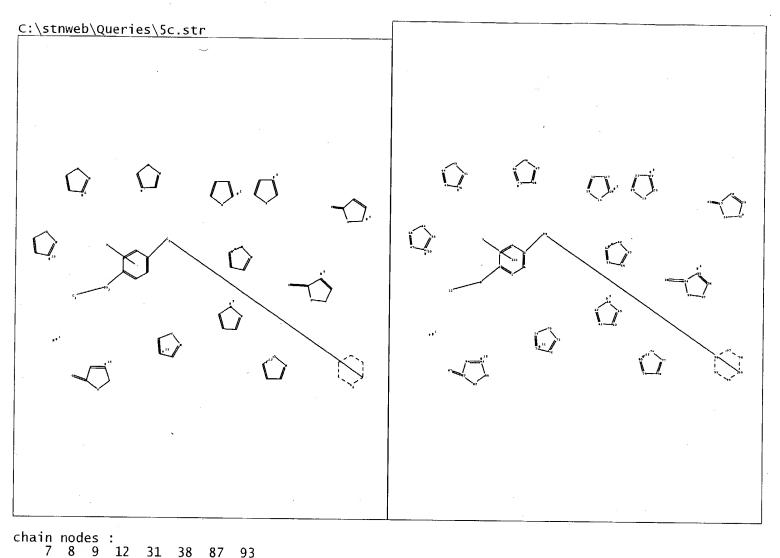
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 101:CLASS

```
C:\stnweb\Queries\5b.str
chain nodes :
   7 8 9 12
                31 38 87
                            93
ring nodes :
               5 6 14
                        15 16 17 18 19 20 21 22 23 26 27 28 29
                                              50 52 53 54 55 56 58 59 60 61 62
77 78 79 80 82 83 84 85 86 94 95
   36
      37
          40
              41 42 43
                          44
                              46
                                  47
                                      48
                                          49
              67
                      70
                           71
                               72
                                   73
                                      74
                                          76
      65
           66
                   68
   96
       97
           98
               99
chain bonds
   2-8 5-93 8-12 27-31 34-38 83-87 93-98
ring bonds :
            2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23
   1-2 1-6
          22-23
                26-27
                       26-30
                              27-28 28-29
                                                   33-34
                                                          33-37
                                            29-30
                                                                 34-35
                                                                         35-36 , 36-37
                                                                                      40-41
   40-44
          41-42
                 42-43
                        43-44
                               46-47
                                      46-50
                                            47-48
                                                    48-49
                                                           49-50
                                                                         52-56
                                                                                      54-55
                                                                 52-53
                                                                               53-54
   55-56
          58-59
                 58-62
                        59-60
                               60 - 61
                                                                        67-68
                                      61-62
                                             64-65
                                                    64-68
                                                          65-66
                                                                 66-67
                                                                               70-71
                                                                                      70 - 74
   71-72
          72-73
                 73-74
                        76-77
                               76-80
                                      77-78
                                            78-79
                                                   79-80
                                                          82-83
                                                                 82-86
                                                                        83-84
                                                                               84-85
                                                                                      85-86
   94-95
          94-99
                95-96
                        96-97
                               97 - 98
                                      98-99
exact/norm bonds :
   2-8 5-93 8-12
                    26-27
                27-28
          26-30
                                                   33-37
                                                                 34-38
                                                                               36-37
                                                                                      40 - 41
   40-44
                 42-43
                                            47-48
                                                    48-49
          41-42
                        43-44
                               46-47
                                      46-50
                                                                                      54-55
70-74
                                                          49-50
                                                                 52-53
                                                                         52-56
                                                                               53-54
          58-59
                 58-62
   55-56
                        59-60
                               60-61
                                             64-65
                                                    64 - 68
                                      61-62
                                                          65-66
                                                                        67-68
                                                                               70-71
                                                                 66-67
                                      77-78
   71-72
          72 - 73
                 73-74
                        76-77
                               76-80
                                            78-79
                                                   79-80
                                                          82-83
                                                                 82-86
                                                                        83-84
                                                                               83-87
                                                                                      84-85
          93 - 98
                94-95
                       94-99
   85-86
                              95-96
                                      96 - 97
                                            97~98
                                                   98 - 99
normalized bonds :
   1-2 1-6 2-3
                 3-4 4-5
isolated ring systems :
   containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :
G1:CH3,Et,[*1]
```

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

33:C,N

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom 73:Atom 74:Atom 76:Atom 76:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom 99:Atom 101:CLASS



```
ring nodes :
                    6
                       14
                           15
                               16 17 18 19 20 21 22 23 26 27
                                                                            29
                                                                        28
                                                                                 30
                                                                                     33
                                                                                         34 35
                    42 43 44 46
                                         48
                                             49
                                                 50 52 53 54 55 56 58 59 60 61 62
     36
            40
                 41
                                     47
       65
            66
    64
                67
                     68
                         70
                             71
                                72
                                     73
                                         74
                                             76
                                                 77
                                                     78
                                                          79
                                                              80 82
                                                                      83
                                                                          84
                                                                               85
                                                                                   86
                                                                                           95
    96 97
                99
            98
chain bonds:
               8-12 27-31 34-38 83-87 93-99
    2-8 5-93
ring bonds :
    1-2 1-6
             2~3
                   3-4
                        4-5 5-6 14-15
                                          14-18 15-16 16-17 17-18
                                                                      19-20
                                                                              19-23
                                                                                     20-21
                                27-28
    21-22
           22-23
                  26-27
                          26-30
                                        28-29
                                                       33-34
                                               29-30
                                                              33 - 37
                                                                     34-35
                                                                             35-36
                                                                                    36-37
                                                                                           40-41
    40-44
                   42-43
           41-42
                          43-44
                                 46-47
                                        46-50
                                               47-48
                                                       48 - 49
                                                              49-50
                                                                     52-53
                                                                             52-56
                                                                                    53-54
                                                                                           54-55
    55-56
            58-59
                   58~62
                          59-60
                                 60 - 61
                                        61-62
                                               64 - 65
                                                       64 - 68
                                                              65-66
                                                                     66-67
                                                                             67-68
                                                                                    70-71
                                                                                           70 - 74
    71-72
           72 - 73
                   73-74
                          76-77
                                 76-80
                                        77-78
                                               78-79
                                                       79-80
                                                              82-83
                                                                     82-86
                                                                            83-84
                                                                                    84-85
                                                                                           85-86
           94-99
    94-95
                  95-96
                          96 - 97
                                 97 - 98
                                        98-99
exact/norm bonds :
    2-8 5-93 8-12
                     14-15
                            14-18
                                   15-16 16-17 17-18 19-20 19-23
                                                                        20-21 21-22
                  27-28
    26-27
           26-30
                          27-31
                                 28-29
                                        29-30
                                               33-34
                                                       33 - 37
                                                              34-35
                                                                     34 - 38
                                                                             35-36
                                                                                    36 - 37
                                                                                           40-41
    40-44
           41 - 42
                  42-43
                          43-44
                                 46-47
                                        46-50
                                               47-48
                                                       48-49
                                                              49-50
                                                                     52-53
                                                                             52-56
                                                                                    53-54
                                                                                           54-55
    55-56
           58-59
                  58-62
                          59-60
                                 60 - 61
                                        61-62
                                               64-65
                                                       64-68
                                                              65-66
                                                                            67-68
                                                                     66 - 67
                                                                                    70-71
                                                                                           70 - 74
           72-73
    71 - 72
                  73-74
                          76-77
                                 76-80
                                        77-78
                                               78-79
                                                       79-80
                                                              82-83
                                                                     82-86
                                                                            83-84
                                                                                    83-87
                                                                                           84 - 85
    85-86
           93-99
                  94 - 95
                         94-99
                                 95-96
                                        96 - 97
                                               97 - 98
                                                       98 - 99
normalized bonds:
    1-2 1-6 2-3
                   3-4 4-5 5-6
isolated ring systems:
    containing 1: 14: 19: 26: 33: 40: 46: 52: 58: 64: 70: 76: 82:
G1:CH3,Et,[*1]
G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]
```

G3:C,N

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 101:CLASS

```
chain nodes :
    7 8 9 12
                 31
                     38
                          87
                              93
ring nodes :
       2
                   6
                      14
                          15
                               16 17 18 19 20 21 22 23 26 27 28
                                                                            29
                                                                                 30
                                                                                     33
                                                                                          34 35
        37
                                         48 49 50 52 53 54 55 56 58 59 60 61 62
74 76 77 78 79 80 82 83 84 85 86 94 95
    36
            40
                41
                    42
                        43
                            44
                                 46 47
       65
    64
            66
                67
                     68
                         70
                             71
                                 72
                                     73
                                                                       83 84
                                                                                   86
    96 97
                99
           98
chain bonds
    2-8 5-93
               8-12 27-31 34-38 83-87 93-96
ring bonds :
                        4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23
    1-2 1-6
             2-3
                  3-4
                                                                                      20-21
           22-23
    21-22
                  26-27
                          26-30
                                 27-28
                                        28-29 29-30
                                                       33-34
                                                              33-37
                                                                      34-35
                                                                             35-36
                                                                                     36-37
                                                                                            40-41
    40-44
           41-42
                  42 - 43
                                                              49-50
                          43-44
                                 46-47
                                        46 - 50
                                                47-48
                                                       48-49
                                                                      52-53
                                                                             52-56
                                                                                     53-54
                                                                                            54-55
    55-56
           58-59
                  58-62
                          59-60
                                 60-61
                                        61 - 62
                                                64 - 65
                                                       64 - 68
                                                              65-66
                                                                      66-67
                                                                             67-68
                                                                                     70-71
                                                                                            70-74
    71-72
           72-73
                  73-74
                          76-77
                                 76-80
                                        77-78
                                                78-79
                                                       79-80
                                                              82-83
                                                                      82-86
                                                                             83-84
                                                                                     84 - 85
                                                                                            85-86
    94 - 95
           94 - 99
                  95-96
                          96 - 97
                                 97 - 98
                                        98-99
exact/norm bonds
    2-8 5-93 8-12
                     14-15
                           14-18
                                    15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23
```

G1:CH3,Et,[*1]
G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]
G3:C,N

28-29

46-47

60-61

76-80

95-96

29-30

46-50

61-62

77-78

96-97

containing 1: 14: 19: 26: 33: 40: 46: 52: 58: 64: 70: 76: 82:

33-34

47-48

64-65

78-79

97 - 98

33-37

48-49

64-68

79-80

98-99

34 - 35

49-50

65 - 66

82-83

34-38

52-53

66 - 67

82-86

35-36

52-56

67-68

83-84

36 - 37

53-54

70-71

83-87

40-41

54-55

70-74

84-85

27-28

42-43

58-62

73-74

94-95

27-31

43-44

59-60

76-77

94-99

3-4 4-5 5-6

26-27

40-44

55-56

71-72

85-86

1-2

normalized bonds :

26-30

41-42

58-59

72-73

93 - 96

1-6 2-3

isolated ring systems:

C:\stnweb\Queries\1.str

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom 99:Atom 101:CLASS

```
C:\stnweb\Queries\4.str
chain nodes :
   7 8 9
            12
               31
                   38 87 93
ring nodes :
               5 6 14
                         15 16 17 18 19 20 21 22 23 26 27 28 29
   1 2 3
                                                                               30 33 34 35
   36 37
           40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
       65
                                               77 78 79 80 82 83 84 85 86
           66
               67
                   68 70
                            71
                               72
                                   73 74 76
       97
           98
               99
   96
chain bonds
   2-8 5-93 8-12 27-31 34-38 83-87 93-95
ing bonds
                      4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23
7 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36
   1-2 1-6
            2-3 3-4
                                                                                    20-21
          22-23
                 26-27
                                                                                   36-37
   40-44
                  42-43
                         43-44
          41-42
                                46-47
                                       46-50
                                              47-48
                                                     48-49
                                                             49-50
                                                                    52-53
                                                                            52-56
                                                                                          54-55
                                                                                   53-54
   55-56
                                       61-62
77-78
          58-59
                 58-62
                         59-60
                                60-61
                                              64-65
                                                      64-68 . 65-66
                                                                    66-67
                                                                           67-68
                                                                                          70-74
                                                                                   70-71
                                              78-79
   71-72
          72 - 73
                 73-74
                        76-77
                                76-80
                                                     79-80 82-83
                                                                    82-86
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                                                                                   84-85
                                                                                          85-86
   94-95
                 95-96
                        96-97
                                       98-99
          94-99
                                97 - 98
exact/norm bonds
   2-8 5-93 8-12
                   14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23
          26-30
                 27-28
                        27-31
                                28-29 29-30
                                              33-34
                                                      33-37
   26-27
                                                             34~35
                                                                    34-38
                                                                            35 - 36
                                                                                   36-37
                                                                                          40-41
   40-44
                 42-43
                                                                    52-53
          41-42
                        43-44
                                46-47
                                       46-50
                                              47-48
                                                      48-49
                                                             49-50
                                                                            52-56
                                                                                          54-55
                                                                                   53-54
                         59-60
                                       61-62
77-78
                                              64-65
                                                             65-66
   55-56
          58-59
                 58-62
                                60-61
                                                      64 - 68
                                                                    66-67
                                                                           67-68
                                                                                   70-71
                                                                                          70 - 74
                 73-74
   71-72
          72-73
                        76-77
                                              78 - 79
                                                      79-80
                                76-80
                                                             82-83
                                                                    82-86
                                                                           83-84
   85-86
          93-95
                 94-95
                        94-99
                                95-96
                                       96-97
                                              97-98
                                                      98 - 99
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6
solated ring systems:
   containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :
51:CH3,Et,[*1]
```

52:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

3:c,N

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 55:Atom 59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 101:CLASS

```
C:\stnweb\Queries\9.str
chain nodes :
     7 8 9 12 31 38 87 93
ring nodes :
     1 2 3 4 5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35 36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62 64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86
```

```
chain bonds :
   2-8 5-93 8-12 27-31 34-38 83-87
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 4
                                                                                 52-56
                                                                          52-53
    40-44
           41-42
                   42-43
                          43-44
                                  46-47
                                          46-50
                                                 47-48
                                                          48-49
                                                                 49-50
                                                                                         53-54
                                                                                                 54-55
                  58-62 59-60
73-74 76-77
                                                                                         70-71
                                                                                                 70-74
                                                  64-65
                                                          64-68 65-66
                                                                          66-67
                                                                                 67-68
    55-56
           58-59
                                   60-61
                                          61 - 62
                                   76-80
                                                  78-79
                                                         79-80 82-83
                                                                          82-86
                                                                                 83-84
                                                                                         84-85
                                                                                                 85-86
                                          77-78
    71-72
           72-73
exact/norm bonds :
    5-93 8-12 27-31 34-38 40-41 40-44 41-42 46-47 46-50 47-48 52-53 52-56 53-54
    58-59 58-62 59-60 65-66 71-72 77-78 83-87
exact bonds :
    2-8 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27 26-30
    27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 42-43 43-44 48-49 49-50 54-55 55-56 60-61 61-62 64-65 64-68 66-67 67-68 70-71 70-74 72-73 73-74 76-77 76-80
    55-56 60-61 61-62 64-65 64-68 66-67
           79-80 82-83 82-86 83-84 84-85 85-86
    78-79
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems:
    containing 1: 14: 19: 26: 33: 40: 46: 52: 58: 64: 70: 76: 82:
G1:CH3,Et,[*1]
G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS

Match level

14:Atom

	15:Atom	16:Atom	17:Atom	18:Atom	19:Atom	20:Atom	21:Atom	22:Atom	23:Atom
26:Atom	27:Atom	28:Atom	29:Atom	30:Atom	31:CLASS	33:Atom	34:Atom	35:Atom	36:Atom
37:Atom	38:CLASS	40:Atom	41:Atom	42:Atom	43:Atom	44:Atom	46:Atom	47:Atom	48:Atom
49:Atom	50:Atom	52:Atom	53:Atom	54:Atom	55:Atom	56:Atom	58:Atom	59:Atom	60:Atom
61:Atom	62:Atom	64:Atom	65:Atom	66:Atom	67:Atom	68:Atom	70:Atom	71:Atom	72:Atom
73:Atom	74:Atom	76:Atom	77:Atom	78:Atom	79:Atom	80:Atom	82:Atom	83:Atom	84:Atom
85:Atom	86:Atom	87:CLASS	93:CLAS9	5 94:CLAS	55				

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